

Model Performance

Model	Data
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Weighted KNN model					
5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 1.79

Global applicability domain: Inside

Local applicability domain index: 3.34e-01

Confidence level: 7.70e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Trimethyl phosphate</div> <div>Measured: 1.41</div> <div>Predicted: 1.50</div>	<div>Image not found</div> <div>Triethyl phosphate</div> <div>Measured: 1.29</div> <div>Predicted: 1.38</div>	<div>Image not found</div> <div>Melamine</div> <div>Measured: 3.80</div> <div>Predicted: 2.45</div>
<div>Image not found</div> <div>Benzenesulfonamide</div> <div>Measured: 4.79</div> <div>Predicted: 2.10</div>	<div>Image not found</div> <div>Triisopropanolamine</div> <div>Measured: 5.75e-01</div> <div>Predicted: 7.42e-01</div>	